Kalman Filtering for Data Assimilation in Linear Systems with Negligible Process Noise: State and Boundary Conditions Estimation

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Abstract

Initial conditions, boundary conditions, state estimation problems are often encountered in data assimilation. Control theory techniques can be adapted to solve such problems, such as Kalman filtering. For systems with a relatively small order the Kalman filtering provides an optimal solution to many data assimilation problems. However, for large scale systems that arise from discretizing partial differential equations, the number of computations and the required storage for the Kalman filter become prohibitive. Also numerical difficulties may arise from propagation of errors, due to finite machine precision computations. Often they result in the violation of the requirement that the error covariance matrix should be positive semi-definite. In this paper we will discuss a Singular Square Root Algorithm (SSQR) to compute a Kalman filter gain for large scale systems, which solves in a reasonable manner the problems mentioned above when the process noise can be assumed to be negligible.

Keywords: Data Assimilation, Kalman Filter, Process Noise, Boundary conditions.

1 Introduction

Complex processes can be often simulated efficiently by systems of discretized partial differential equations describing the conservation laws. The discretized system of equations provides a reasonably accurate forecast of the future dynamical behaviour, provided that the initial state of the system and the boundary conditions are known. However, for real application a complete information defining the state of the system at a specific time is seldom available. Moreover, both the models and the measured data contain inaccuracies and random noise. Observations of the system measured over an interval of time can be used in combination with the model equations to derive estimates of the expected values of the physical states. The problem of constructing a state-estimator for these systems can be treated by using feedback design techniques from control theory like Kalman filtering [6]. Although Kalman filter has shown to provide an optimal solution for linear systems with a relatively small order, for very large nonlinear systems it is not directly applicable, because its computation complexity. As a result, approximations of the Kalman filter equations are needed.

Following Todling and Cohn [10] we will refer to these approximations suboptimal schemes or SOS's.

Most SOS's are aimed at an approximation of either the model dynamics or the error covariance matrix, due to the fact that the main part of the computations are used for them. The model is often simplified by removing less important terms from the equations, or by introducing other simplifying assumptions. The simplified model is then used for time propagation of the error covariance and the full model for the time propagation of the estimate. Some researchers [3], have proposed to approximate the state transition matrix by one of the lower rank. The partial singular value decomposition can be used in this case to reduce the computations.

Various methods have been proposed for the approximation of the error covariance matrix. Setting correlations for large distances to zero can be exploited to speed the algorithm up considerably. However, due to the generally large condition number of the error covariance matrix negative eigenvalues may appear. A solution to this problem is to use

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a square root filter [8]. Often the error covariance matrix has only a few large eigenvalues, which can be used for approximation. The resulting partial eigenvalue decomposition can be used for fast propagation of the error covariance. Todling and Cohn used this idea together with a Lanczos algorithm for the eigenvalue computations to obtain an efficient and general algorithm, the Partial Eigen-decomposition Kalman Filter or PEKF [3]. Another similar idea by Verlaan and Heemink is to approximate the error covariance matrix by one of a lower rank, the Reduced Rank Square Root algorithm or RRSQRT-KF [12]. The optimal choice for this low rank approximation results in the use of the eigenvalues and eigenvectors of the error covariance matrix.

In this paper we will discuss a Singular Square Root Filter algorithm to compute a Kalman Filter gain or SSQRT-KF algorithm for large scale systems. Assuming a perfect model, no process noise, it is possible to compute a Kalman filter gain at a very low computational cost using the classical square root algorithm [8]. Even though this filter is not optimal, it guarantees that the estimation error will converge to zero by relocating the most dominant eigenvalues of the error estimation transition matrix. Nevertheless, there is a design parameter r that can be adjusted to obtain a better performance of the filter.

Besides of that, another problem are the boundary conditions. Due to the fact that we are dealing with first principle based models, it is very important to know the initial and boundary conditions of the system in order to make a more reliable estimation and prediction of the states. Boundary conditions can be assumed to be unknown inputs, in that case, it is possible to use an augmented state space system to estimate the boundary conditions. In this paper we will show how to invert a linear dynamic system using a Kalman filter formulation [11] in order to estimate the boundary conditions.

This paper is organized as follows. In the second section, a problem formulation is given. In the third and fourth sections, the discrete Kalman filter and the Discrete Riccati Difference Equation are presented. Fifth section is dedicated to introduce the new algorithm SSQRT-KF. In the sixth section, the RRSQRT-KF algorithm is described. Finally, in the last section a comparison between the full Kalman, RRSQRT-KF and SSQRT-KF filters is done, taking a heat transfer systems in an insulated plate as example.

2 Problem Formulation

A discretized linear PDE can be written as a state space representation of an LTV stochastic model as follows:

$$x_{k+1} = A_k x_k + B_k u_k + w_k, \quad (1)$$
$$y_k = C x_k + v_k. \quad (2)$$

where $A_k \in \mathbb{R}^{n\times n}$, $B_k \in \mathbb{R}^{n\times p}$ and $C_k \in \mathbb{R}^{m\times n}$ with $n \gg m, p$. Additionally we have

$$\begin{aligned} E[w_j w_k^T] &= Q_k \delta_{jk}, \\ E[v_j v_k^T] &= R_k \delta_{jk}, \\ E[v_j w_k^T] &= 0, \end{aligned} \quad (3)$$

where $E[.]$ denotes expectation, w_k is a white Gaussian system noise process with zero mean and covariance matrix Q_k which is introduced to take into account model uncertainties like missing or erroneous physics, and computation errors, as well as the white Gaussian measurement noise process v_k with zero mean and covariance matrix R_k to take into account the measurements uncertainties. The initial state x_0 is assumed to be Gaussian with zero mean and covariance matrix P_0. The initial conditions, the system and measurements noise processes are all assumed to be independent of each other.

Moreover, for data assimilation models the probability density function of the states can be determined based on the history of the measurements $y_1, \ldots, y_k$. For the model (2) it can be shown that this conditional density function is Gaussian. Therefore it is completely characterized by its mean and covariance matrix. Furthermore, for a Gaussian distribution, the mean is an optimal estimate in a maximum likelihood sense, via a least squares estimation.

Having defined the general stochastic state space representation of the model (1) and the measurement relation (2), it is desired to combine the measurements with the information provided by the model to obtain an optimal estimate of the system states, this problem is called a filtering problem. For solving this problem the Kalman filtering (KF) will be used.

3 Discrete Time Kalman Filter

The problem of estimating the states of (1) from measurements of the output (2) is discussed in this section. Different estimators can be derived depending on the available measurements. Assuming that the data

$$\mathbf{Y}_k = \{y_i, u_i | i \leq k\}$$

is known, then, by using $\mathbf{Y}_k$ we want to estimate x_{k+k_m}. There are three distinct cases:

1. Smoothing ($k_m < 0$)
2. Estimation (Filtering) ($k_m = 0$)
3. Prediction ($k_m > 0$)

Figure 1 illustrates the different cases. In the next section the estimation problem is discussed. The resulting dynamic system is called a filter regardless of which of the problems is solved. We refer to [1] for the proofs of the results given in this section.

3.1 Estimation Problem

A estimation of the signal x_k is concerned with the estimation of x_{k+k_m} for $k_m = 0$ using the measurements y_i for $0 \leq i \leq k$. Consider the discrete-time dynamical system described by (1) and (2). For this system, we take a state estimator of the form

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k(y_k - \hat{y}_{k|k-1}), \quad k \geq 0, \tag{4}$$

where $L_k \in \mathbb{R}^{n \times m}$, with output

$$\hat{y}_{k|k-1} = C_k \hat{x}_{k|k-1}. \tag{5}$$

The first step of the recursive procedure is to propagate ahead $x_{k-1|k-1}$ via (1)

$$\hat{x}_{k|k-1} = A_{k-1} x_{k-1|k-1} + B_{k-1} u_{k-1}, \tag{6}$$

then, define the prior state estimation error by

$$e_{k|k-1} \triangleq x_k - \hat{x}_{k|k-1},\ k > 0. \tag{7}$$

Substituting (6) and (1) into (7) we obtain

$$e_{k|k-1} = A_{k-1} e_{k-1|k-1} + w_{k-1}, \tag{8}$$

now, define the prior error covariance matrix by

$$P_{k|k-1} \triangleq E[e_{k|k-1} e_{k|k-1}^T], \tag{9}$$

hence,

$$P_{k|k-1} = A_{k-1} P_{k-1|k-1} A_{k-1}^T + Q_{k-1}. \tag{10}$$

Next, define the state estimator error

$$e_{k|k} \triangleq x_k - \hat{x}_{k|k}, \tag{11}$$

consequently, the Kalman gain L_k minimizes

$$J_k(L_k) = tr(P_{k|k}), \tag{12}$$

where the estimation error covariance matrix $P_{k|k} \in \mathbb{R}^{n \times n}$

$$P_{k|k} \triangleq E[(e_{k|k} - E[e_{k|k}]])(e_{k|k} - E[e_{k|k}])^T]. \tag{13}$$

As a result, the Kalman gain can be obtained by

$$L_k = P_{k|k-1} C_k^T \hat{R}_k^{-1}, \tag{14}$$

where $\hat{R}_k \in \mathbb{R}^{m \times m}$ is defined by

$$\hat{R}_k = R_k + C_k P_{k|k-1} C_k^T. \tag{15}$$

The error covariance matrix update

$$P_{k|k} = (I_n - L_k C_k) P_{k|k-1}. \tag{16}$$

4 Square Root Kalman Filter Formulation

To compute more efficiently the Kalman filter gain, we are going to use the recursive square root algorithm proposed by Moore and Kailath [8].

To derive the square root form of the Kalman filter, first assume that the Cholesky factorization of the positive semi-definite matrices R_k, Q_{k-1}, and $P_{k|k-1}$ are defined by

$$R_k \triangleq L_{R_k} L_{R_k}^T, \tag{17}$$

$$Q_{k-1} \triangleq L_{Q_{k-1}} L_{Q_{k-1}}^T, \tag{18}$$

$$P_{k|k-1} \triangleq S_{k|k-1} S_{k|k-1}^T. \tag{19}$$

Where $S_{k|k-1}$ is defined as

$$S_{k|k-1} \triangleq \left[A_{k-1} S_{k-1|k-1} L_{q_{k-1}} \right]. \tag{20}$$

Next,notice that the Schur complement of the block $\hat{R}_k$ in (21) is (16),

$$M_k = \begin{pmatrix} \hat{R}_k & C_k P_{k|k-1} \\ P_{k|k-} C_k^T & P_{k|k-1} \end{pmatrix}. \tag{21}$$

Then, M_k is easily factorized in:

$$Mk = \begin{pmatrix} L_{R_k} & C_k S_{k|k-1} \\ 0 & S_{k|k-1} \end{pmatrix} \begin{pmatrix} L_{R_k}^T & 0 \\ S_{k|k-1} C_k^T & S_{k|k-1}^T \end{pmatrix} \tag{22}$$

Now, the so-called square root form is obtained from a lower triangular reduction or QR decomposition of the left factor as follows

$$\begin{pmatrix} L_{R_k} & C_k S_{k|k-1} \\ 0 & S_{k|k-1} \end{pmatrix} \cdot U_k = \begin{pmatrix} H_k & 0 \\ J_k & S_{k|k} \end{pmatrix}, \tag{23}$$

where U_k is orthogonal. As a consequence, a square root factorization of M_k is yielded by

$$M_k = \begin{pmatrix} H_k & 0 \\ J_k & S_{k|k} \end{pmatrix} \begin{pmatrix} H_k^T & J_k^T \\ 0 & S_{k|k}^T \end{pmatrix}, \tag{24}$$

from which it follows that $P_{k|k} = S_{k|k} S_{k|k}^T$. Notice that this holds even if $P_{k|k}$ is not full rank.

Finally, the Kalman gain can be computed as

$$L_k = J_k (H_k)^{-1}. \tag{25}$$

Summarizing, the recursive Kalman filter algorithm will be as follows

1. Update

$$\hat{x}_{k|k-1} = A_{k-1} \hat{x}_{k-1|k-1} + B_{k-1} u_{k-1}$$

2. Update

$$S_{k|k-1} = \left[A_{k-1} S_{k-1|k-1} L_{Q_{k-1}} \right]$$

3. Compute $S_{k|k}$ and L_k from (24) and (25) respectively.

4. Compute

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k (y_k - C_k \hat{x}_{k|k-1}).$$

5 SSQR Kalman Filter Algorithm (SSQRT-KF)

In the case of the state estimation for large scale systems, the computational complexity in (20), (23) is still too large. However, it is possible to explore the freedom of some parameters to derive low-rank algorithms. In this section we describe an algorithm that we call the Singular Square Root Kalman Filter (SSQRT-KF) , which is able to compute a suboptimal Kalman filter gain very efficiently, assuming the process noise covariance $Q_{k-1} = 0$. It is inspired for a dual algorithm described in [13].

In [13] is shown that for LTI systems the spectrum of the state space observer dynamics matrix $A(I_n - P_{k|k-1}C^T\hat{R}^{-1}C)$ is the union of the spectrum of A and that of A^{-1} for the case $Q = 0$. Moreover, it is also shown for the same case that the rank of the steady state error covariance matrix $P_{k+1|k}$ is equal to the dimension of the unstable subspace of A. Even though this results were developed for the dual algorithm of the state prediction problem, the results can be directly extended to the state estimation case due to the fact that the eigenvalues of the error dynamics matrix in the two cases; prediction and estimation, can be shown to be the same. Hence (20) can be written as

$$S_{k|k-1} \triangleq A_{k-1}S_{k-1|k-1}, \tag{26}$$

where the $S_{k|k-1} \in \mathbb{R}^{n\times l}$, with l chosen larger than the number of unstable eigenvalues of A. Then, notice that the QR decomposition is computed for a small matrix of size $(p + l) \times p$ making it cheap to compute. On the other hand, if the measurements are uncorrelated, i.e., R diagonal, then $\hat{F}_k$ will be diagonally dominant, therefore instead of computing $\hat{F}_k^{-1}$, we invert its diagonal entries to obtain a diagonal approximation of F_k^{-1}. Besides, if C is sparse, the construction of the left factor in the left hand side of (23) is cheap as well.

A key characteristic of SSQRT-KF algorithm is that the spectrum of the state space observer dynamics matrix $(I_n - P_{k|k-1}C^T\hat{R}^{-1}C)A$ is constructed by reflecting the eigenvalues of A with $|\lambda| > 1$ to their unit circle mirror images $1/|\lambda|$, and leaving the eigenvalues with $|\lambda| < 1$ unchanged.

Summarizing, the recursive SSQRT-KF algorithm will be as follows

1. Update
$$\hat{x}_{k|k-1} = A_{k-1}\hat{x}_{k-1|k-1} + B_{k-1}u_{k-1}.$$
2. Update
$$S_{k|k-1} = A_{k-1}S_{k-1|k-1}.$$
3. Compute $S_{k|k}$ and L_k from (23) and (25) respectively.
4. Compute
$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k(y_k - C_k\hat{x}_{k|k-1}).$$

6 Reduced Rank Square Root Kalman Filter (RRSQRT-KF) [12]

In the RRSQRT-KF estimator the square root factors are based on an eigendecomposition. Let $P_{k|k-1} = V_k\Lambda_kV_k^T$ be the eigendecomposition of the error covariance matrix $P_{k|k-1}$, so that $S_{k|k-1} = V_k\Lambda_k^{1/2}$ is a square root factor of $P_{k|k-1}$. The error covariance matrix is now approximated by using only q leading eigenvalues. With the ordering $|\lambda_1| \geq \ldots \geq |\lambda_n| \geq 0$, an approximation is obtained by truncating $S_{k|k-1}$ after the first q columns. The algorithm is as follows:

1. Update $\hat{x}_{k|k-1} = A_{k-1}\hat{x}_{k-1|k-1} + B_{k-1}u_{k-1}$
2. Update $S_{k|k-1} = [A_{k-1}S_{k-1|k-1} \ L_{Q_{k-1}}]$
3. Rank reduction of the error covariance:
$$S^*_{k|k-1} = [S_{k|k-1} \ V_k]_{1:n,1:q},$$
where
$$S^T_{k|k-1}S_{k|k-1} = V_k\Lambda_kV_k^T$$
4. Compute L_k and $S_{k|k}$ using the scalar update of Potter [7] for independent measurements as follows,
$S_{k|k} = S^*_{k|k-1}$,
for $i = 1$ to p,
$$\begin{aligned} H &= S^{*T}_{k|k-1}C_k(i,:)^T \\ F &= (H^TH + R_k(i,i))^{-1} \\ L_k(:,i) &= S^*_{k|k-1}HF \\ S_{k|k} &= S_{k|k} - L_kH^T(1 + (FR_k(i,i))^{1/2})^{-1}. \end{aligned}$$
end
5. Compute $\hat{x}_{k|k} = \hat{x}_{k|k-1} + L_k(y_k - C_k\hat{x}_{k|k-1})$

If the measurements are correlated, i.e., R_k is not diagonal then these measurements can be transformed. Let $\tilde{y}_k$ be defined by

$$\tilde{y}_k \triangleq R_k^{-1/2}y_k, \tag{27}$$

where $R_k^{-1/2}$ is the matrix inverse of the Cholesky factor of R_k. Then

$$\tilde{y}_k = \tilde{C}_kx_k + \tilde{v}_k, \tag{28}$$

with,

$$\tilde{C}_k \triangleq R_k^{-1/2} C_k, \quad (29)$$

$$\tilde{v}_k \triangleq R_k^{-1/2} v_k. \quad (30)$$

These transformed measurements are equivalent to the original measurements, but the covariance matrix of the errors of $\tilde{v}_k$ is the identity matrix.

The number of computations required in the time propagation of the error in the covariance, which is a major fraction of the total number, is reduced by a factor n/q with respect to the original Kalman filter algorithm. It can be shown that for $q = n$ the RRSQRT-KF algorithm is exact in the sense that it is equivalent to the Kalman filter equations. The parameter q controls the accuracy of the approximation. The price for greater accuracy is as always a larger computational burden.

7 Numerical Results

As an example, a heat transfer system in an finite insulated plate will be taken. The PDE which describes such a system [5] is given by

$$\frac{\partial T(t,y,x)}{\partial t} = \alpha \left(\frac{\partial^2 T(t,y,x)}{\partial x^2} + \frac{\partial^2 T(t,y,x)}{\partial y^2} \right) + u(t,y,x), \quad (31)$$

where $T(t,y,x)$, $u(t,y,x)$, and α are the temperature distribution, the heat input, and the heat transfer coefficient of the plate, respectively. In this example the PDE is discretized using finite differences, with the plate dimensions $L_x = L_y = 1m$, $\alpha = 1 \times 10^{-5} W/^oCm^2$, with fixed boundary conditions, initial conditions

$$T(0,y,x) = 0,$$

and the heat input

$$u(t,y,x) = 5 \times 10^{-5} \frac{\Delta t}{\Delta x} e^{\frac{-(x-x_0(t))^2}{2\sigma_x} + \frac{-(y-y_0(t))^2}{2\sigma_y}}. \quad (32)$$

Where $x_0(t)$ and $y_0(t)$ are values that change with time, and $\sigma_x = \sigma_y = 1e-2$. The system is discretized in 225 grid points equally spaced by $\Delta x = \Delta y = 0.0625$ with $0 < x < 1$ and $0 < y < 1$, and a sampling time $\Delta t = 5.21sec$, this in order to keep the discretized system stable. Figure 5 shows the structure of the A matrix, this structure is very typical for discretized PDE's. We can observe that this matrix is very sparse which can be used to make the computations more efficient.

For simulation purposes the short range prediction scheme is used. This scheme consist of estimating the states at time k, where the measurements y_k are available, with the Kalman filter. Then, the prediction is done by projecting ahead the states using the physical first principle based model (1) until new measurements are taken.

In a first simulation, 30 measurement points were taken randomly, and the process noise was set to zero. Figure 2 shows a comparison of the RMSE between the three filters for this case. Although the three algorithms converge to the same solution, RRSQRT-KF converges slower while SSQRT-KF have a similar convergence behaviour to the classical KF. In a second simulation process noise was introduced by using just the inputs at the same points where the outputs are measured, using the same 30 measurement points of the previous simulation. The filters were computed assuming no process noise. Figure 3 shows the results of the RMSE, as expected none of the filters converge to zero.

The third simulation was done taking into account the process noise caused by the unknown inputs. The performance of the classical KF and RRSQRT-KF are much better now, while SSQRT-KF keeps the same performance of the previous case due to the fact that it does not take into account the process noise in its formulation, figure 4 shows the results.

In order to improve the performance of the SSQRT-KF when process noise is present in the system, covariance inflation can be applied [2]. The covariance inflation is a heuristic approach used in the ensemble Kalman filter to avoid filter divergence, it consists of multiplying the error covariance matrix $P_{k|k-1}$ by a factor γ ($\gamma > 1$) enlarging the prior distribution artificially. In the SSQRT-KF this γ can be seen as a compensator for the lack of the process noise term in (20). Hence the error covariance update can be rewritten as

$$P_{k|k-1} = \tilde{A}_{k-1} P_{k-1|k-1} \tilde{A}_{k-1} \quad (33)$$

where $\tilde{A}_{k-1}$ is defined by

$$\tilde{A}_{k-1} \triangleq \sqrt{\gamma} A_{k-1}. \quad (34)$$

The chosen of γ has to be done with care, because if γ is chosen too large it results in a filter in which the observation are given too much weight.

Consequently, when it is dealt with discretized PDE systems (1), the matrix A_k is in most of the cases stable, i.e, $|\lambda(A_k)| < 1$. Therefore we can choose γ such that the matrix $\tilde{A}_{k-1}$ gets the most dominant eigenvalues outside the unit circle. Since it was mentioned in §5, one of the key characteristics of the SSQRT-KF is that the spectrum of the state space observer dynamics matrix $A - L_k C$ is constructed by reflecting the eigenvalues of A_k with $|\lambda| > 1$ to their unit circle mirror images $1/|\lambda|$, and leaving the eigenvalues with $|\lambda| < 1$ unchanged. Hence, the SSQRT-KF estimator will focus on the most dominant modes of the system dynamics, obtaining a suboptimal KF.

Figure 6 shows a comparison of RMSE between the three filters when covariance inflation is applied to them. Even though all the filters reduce the RMSE, SSQRT-KF reduces it drastically compare to the others. Figure 7 depicts how the magnitude of the eigenvalue of the filter dynamics are affected compared to the eigenvalues of the system dynamics. At the bottom can be seen for the SSQRT-KF case how $|\lambda(\tilde{A}_{k-1})| > 1$ are moved into the unit circle leaving the rest in their original locations.

Another important feature of the SSQRT-KF algorithm is its low computation cost as can be seen in table (1). There can be seen that for n $\gg$ m,l,q,p RRSQRT and SSQRT-KF are much cheaper to compute than Kalman filter.

8 Boundary Conditions Estimation

Until now boundary conditions were assumed to be zero, but in real applications we often find that this is not true. Therefore, in this section the boundary conditions are added to the system described by (1) and (2). As a result, a discretized PDE with boundary conditions can be set as a LTV stochastic model state space representation as follows:

$$\begin{aligned} x_{k+1} &= A_k x_k + B_k u_k + F_k z_k + w_k && (35)\\ y_k &= C_k x_k + v_k. && (36) \end{aligned}$$

where $A_k \in \mathbb{R}^{n\times n}$, $B_k \in \mathbb{R}^{n\times p}$, $C_k \in \mathbb{R}^{m\times n}$, and $F_k \in \mathbb{R}^{n\times b}$. With $z_k \in \mathbb{R}^b$ a vector of boundary conditions at time k.

$$\begin{aligned} E[w_j w_k^T] &= Q_k \delta_{jk} \\ E[v_j v_k^T] &= R_k \delta_{jk}, \\ E[v_j w_k^T] &= 0 \end{aligned} \quad (37)$$

Where w_k is a white Gaussian system noise process with zero mean and covariance matrix Q_k which is introduced to take into account the model uncertainties, as well as the white Gaussian measurement noise process v_k with zero mean and covariance matrix R_k to take into account the measurements uncertainties. The initial state x_0 is assumed to be Gaussian with mean $\bar{x}_0$ and covariance matrix P_0.

In (35) is seen that the boundary condition vector z_k can be taken as external input to the system. Hence (35) and (36) can be rewritten as follows

$$\begin{aligned} x_{k+1} &= A_k x_k + (B_k \;\; F_k)\begin{pmatrix} u_k \\ z_k \end{pmatrix} + w_k && (38)\\ y_k &= C_k x_k + v_k. && (39) \end{aligned}$$

Now, in order to estimate the boundary conditions vector, we are going to invert the system using the Kalman filter such that the vector z_k will become part of the state space vector x_k, as explained in the following section.

8.1 Inverting Linear Dynamical Systems [11]

As an application of the Kalman filter, in this section we present how Kalman filtering can be used to invert a linear dynamical system. We start with a rather crude problem formulation. Let the signal generating system be described by the LTI formulation of the state space system (35), (36), and let a desired output sequence y_{dk} be given for $k = 1, 2, \ldots, N$. Then the problem is to determine the input sequence z_k for $k = 1, \ldots, N$ such that y_k closely approximates y_{dk}.

A more precise problem formulation requires the definition of a model that describes how the input z_k is generated. Consider the following model representation for the class of inputs

$$z_{k+1} = \alpha z_k + w_{zk}. \quad (40)$$

This model is an AR(1) with w_{zk} a white noise sequence that is independent of w_k and v_k in (35) and (36), and covariance

$$E[w_{zj} w_{zk}^T] = Q_z \delta_{jk}. \quad (41)$$

For the input within this class of signal generating systems the problem is to determine the output covariance matrix $Q_z \in \mathbb{R}^{b\times b}$ and a realization of the input sequence z_k for $k = 1, 2, \ldots, N$, such that the output y_k is a minimum variance approximation of y_{dk}.

The combination of the time-invariant signal generating model and the model representing the class of input signals (40) results in the augmented state space model:

$$\begin{aligned} \begin{pmatrix} x_{k+1} \\ z_{k+1} \end{pmatrix} &= \begin{pmatrix} A & F \\ 0 & \alpha I_b \end{pmatrix}\begin{pmatrix} x_k \\ z_k \end{pmatrix} + \begin{pmatrix} B \\ 0 \end{pmatrix} u_k + \\ &\quad \begin{pmatrix} I_n & 0 \\ 0 & I_b \end{pmatrix}\begin{pmatrix} w_k \\ w_{zk} \end{pmatrix} && (42)\\ y_k &= (C \;\; 0)\begin{pmatrix} x_k \\ z_k \end{pmatrix} + v_k, && (43) \end{aligned}$$

with the process and measurement noise having the following covariance matrix:

$$E\begin{pmatrix} w_k \\ w_{zk} \\ v_k \end{pmatrix}\begin{pmatrix} w_k^T & w_{zk}^T & v_k^T \end{pmatrix} = \begin{pmatrix} Q & 0 & 0 \\ 0 & Q_z & 0 \\ 0 & 0 & R \end{pmatrix}. \quad (44)$$

This augmented state space model has no measurable boundary conditions sequence. A bounded solution of the state error covariance matrix of the Kalman filter of the augmented state space model requires the pair

$$\left\{ \left(\begin{array}{cc} A & F \\ 0 & \alpha I_b \end{array} \right), \left(\begin{array}{cc} C & 0 \end{array} \right) \right\} \quad (45)$$

to be observable. The conditions under which the observability of the original pair (A, C) are preserved are given in the following lemma.

Lemma 1. *Let the pair (A, C) be observable and let for all $\xi \in \mathbb{R}^m : C(A - \alpha I_n)^{-1} F\xi = 0$ if and only if $\xi = 0$, then the pair (45) is observable.*

Proof: By the Popov-Belevitch-Hautus test for checking observability, we have to proof that for all eigenvectors of the system matrix

$$\left(\begin{array}{cc} A & F \\ 0 & \alpha I_b \end{array} \right)$$

denoted as:

$$\left(\begin{array}{cc} A & F \\ 0 & \alpha I_b \end{array} \right) \left(\begin{array}{c} \eta \\ \xi \end{array} \right) = \lambda \left(\begin{array}{c} \eta \\ \xi \end{array} \right) \quad (46)$$

the condition:

$$\left(\begin{array}{cc} C & 0 \end{array} \right) \left(\begin{array}{c} \eta \\ \xi \end{array} \right) = 0, \quad (47)$$

only holds provided $\left(\begin{array}{c} \eta \\ \xi \end{array} \right) \equiv 0$. From the lower part of (46) it follows that: $\xi = 0$ for any λ and α, or $\lambda = \alpha$ for any ξ. With $\xi = 0$ it follows from (46) that $A\eta = \lambda\eta$ and therefore $C\eta$ can only be zero provided that η is zero, since the pair (A, C) is observable. With $\lambda = \alpha$, the top row of (46) reads:

$$(A - \alpha I_n)\eta = -F\xi, \quad (48)$$

hence $C\eta = 0$ implies,

$$C(A - \alpha I_n)^{-1} F\xi = 0 \quad (49)$$

but this can only hold provided that $\xi \equiv 0$.

The condition in lemma 1 on ξ for single-input, single-output LTI systems is equivalent with the fact that the system (A, F, C) does not have zeros in the point $z = \alpha$ of the complex plane. For multivariable systems the condition corresponds to the original system having no so-called transmission zeros in the point $z = \alpha$, see details in [9].

An important design variable for the Kalman filter of the augmented state space model is the covariance matrix Q_z.

The case where the original system has one or more zeros at α or in a circle of radius ε around $z = \alpha$, requires special attention. Different solutions are available to solve this problem. One approach is based on the factorization of rational transfer functions given in [4].

8.2 Numerical Results

In order to investigate how this technique works in a data assimilation problem, the example of section §7 will be taken. The boundaries are fixed to zero except for the left boundary where the disturbance input $z_{k+1} = z_k + w_k$ with $\alpha = 1$ is injected. The new augmented system has 15 new unknown states, corresponding to the boundary conditions of the left side.

Figure 9 shows the RMSE of the three filters when the disturbance input $z_{k+1} = z_k + w_{zk}$ is injected. In this simulation is assumed all the inputs are known, and 30 output measurement points. Covariance inflation is used for SSQRT-KF with $\gamma = 1.05$

Figure 10 shows a contour plot of the performance comparison of the three filters. Even though the classical KF is the best, RRSQRT-KF and SSQRT-KF do a good job in estimating the unknown input disturbance.

9 Conclusions

In this paper a new algorithm to compute a suboptimal Kalman filter -SSQRT-KF- was introduced for the case when the process noise can be assumed to be negligible or zero. This algorithm is cheap to compute compare to the classical KF. It has been tested and compared with the classical KF as well as the RRSQRT-KF obtaining good results. Although, in the case when the process noise in not zero, the covariance inflation factor added some improvement on the estimation of the filters, SSQRT-KF was the one with a major improvement.

One drawback of the SSQRT-KF, when process noise is present in the system, is that the covariance inflation factor γ has to be tuned in a heuristic way.

For the case of estimating the boundary conditions by inverting the system showed to work well for the three filters. However, we need to know or have a good idea of the class of the input signal is coming in through the boundary.

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II (CP/40: TMS and Sustainibility); EU: CAGE; ERNSI; Eureka 2063-IMPACT; Eureka 2419-FliTE; Contract Research/agreements: Data4s, Electrabel, Elia, LMS, IPCOS, VIB.

References

[1] B.D.O. Anderson and J.B. Moore. *Optimal Filtering.* Prentice Hall, 1979.

[2] J. L. Anderson and S. L. Anderson. A monte carlo implementation of the nonlinear filtering problem to produce ensemble assimilations and forecasts. *Monthly Weather Review*, 127:2741–2758, December 1999.

[3] S. Cohn and R. Todling. Approximate data assimilation schemes fo stable and unstable dynamics. *Metereological Society of Japan*, 74:63–75, 1996.

[4] P. Van Dooren. *Rational and polynomial matrix factorizations via recursive pole-zero cancellation*, volume 137, pp. 663-697. Université Catholique de Louvain, 1990.

[5] R. Haberman. *Elementary Applied Partial Differential Equations.* Springer, 3rd edition, 1998.

[6] R. E. Kalman. A new approach to linear filter and prediction theory. *J. Basic. Engr.*, vol. 82D:35–45, 1960.

[7] P. S. Maybeck. Stochastic models, estimation, and control. *Mathematics in science and engineering, Academic Press, New York*, 141(1), 1979.

[8] M. Morf and T. Kailath. Square-root algorithms for least-squares estimation. *IEEE Trans. Aut. Contr.*, AC(20):487–497, 1975.

[9] J. Vandewalle P.Van Overschee, B. De Moor. *Mulitvariable Systems and Identification.* VTK-KULeuven, 2001.

[10] R. Todling and S. Cohn. Suboptimal schemes for atmospheric data assimilation bsed on the kalman filter. *Monthly Weather Review*, 1994.

[11] M. Verhaegen and V. Verdult. *Lecture Notes on Filtering and System Identification: An Introduction.* TUDelft, 2002.

[12] M. Verlaan and A. W. Heemink. Reduced rank square root filters for large scale data assimilation problems. *2nd International Symposium on Assimilation of Observations in Meteorology and Oceanography, World Meteorological Organization*, pages 247–252, march 1995.

[13] K.Gallivan X.Rao and P. Van Dooren. Singular riccati equations stabilizing large-scale systems. *Lin. Alg. Appl.*, 2003.

	Kalman Filter	RRSQRT-KF	SSQRT-KF
flops	$2n^3(m^3/3n^3 + 3m^2/n^2 + m^2/2n^3+2m/n^2+1/n+3)$	$2n^2(6q^3/n^2 + 2q^2/n + 7mq/2n + qm/n^2 + q)$	$2n^2(2m^2/n + 3ml/m + m^2l/n^2 + l^2/n + l)$
$\sim$ flops n $\gg$ m,l,q,p	$6n^3$	$2n^2q$	$2n^2l$

Table 1: Comparison of the computation complexity between Kalman filter, RRSQRT-KF filter, and SSQRT-KF algorithm. In the first row is shown the number of flops needed one iteration. In the second row is shown the number of flops needed for one iterations when $n \gg, l, q, p$.

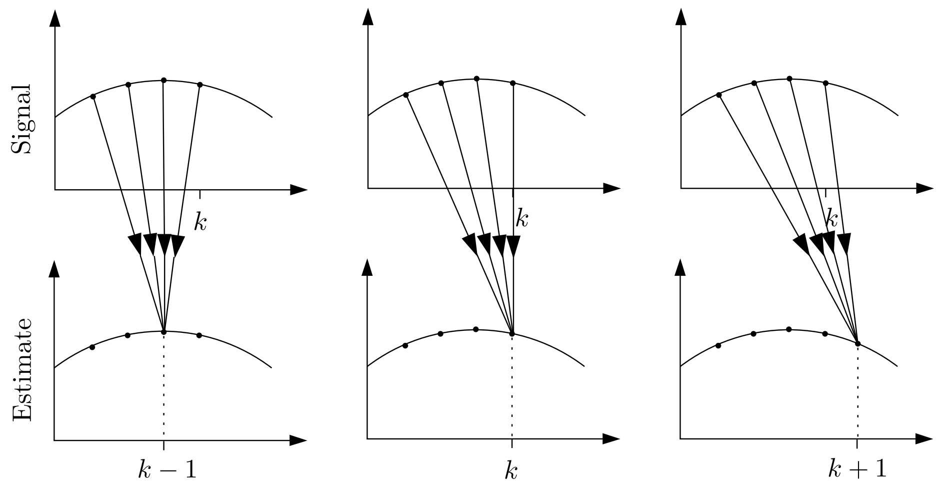

Figure 1: Smoothing, filtering, and prediction

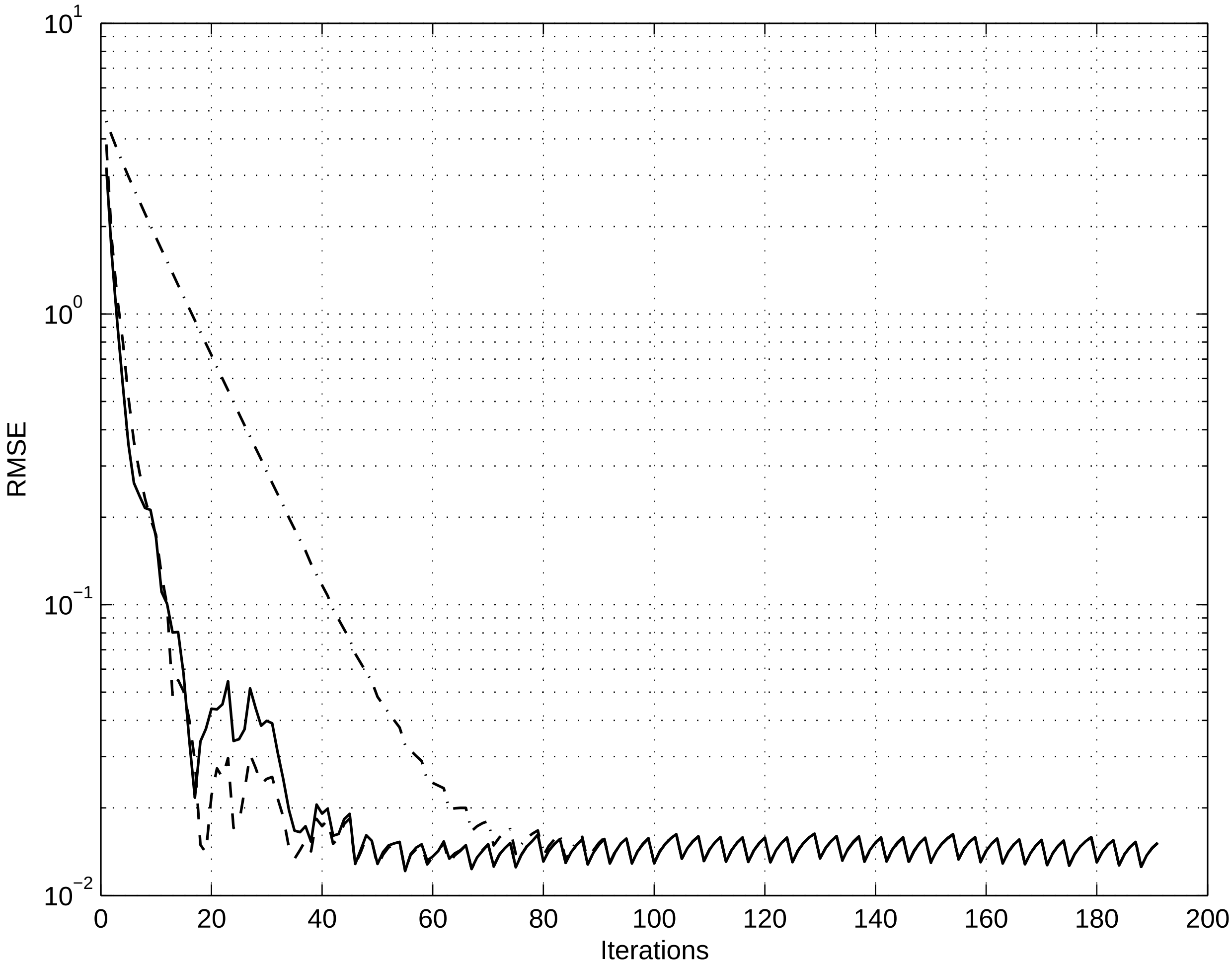

Figure 2: RMSE of $\hat{x}_{k|k}$ for the KF , RRSQRT-KF, and SSQRT-KF, assuming all the inputs known. KF Solid line, RRSQRT-KF dashed-dotted line, and SSQRT-KF dashed line.

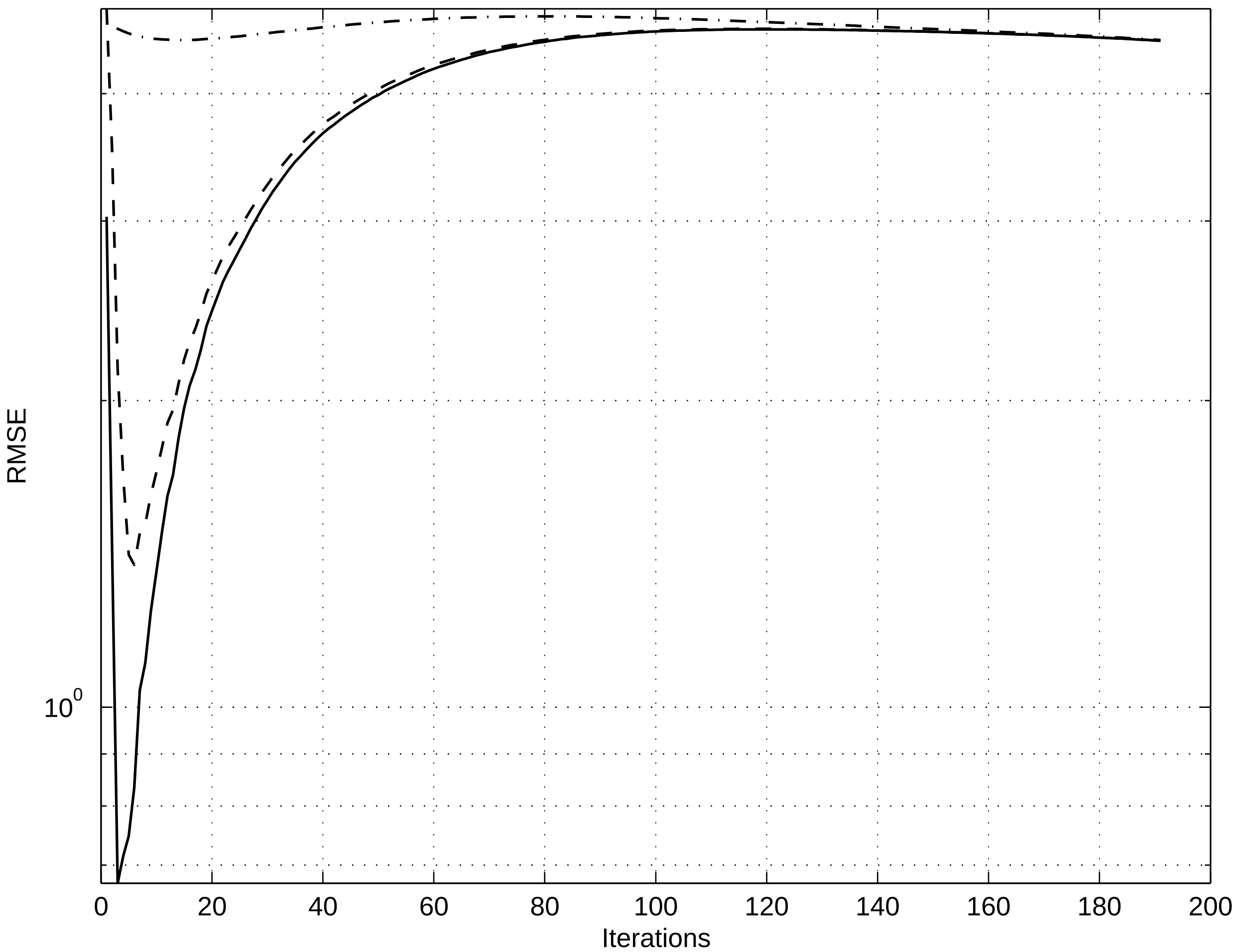

Figure 3: RMSE of $\hat{x}_{k|k}$ for the KF , RRSQRT-KF, and SSQRT-KF, taking just the inputs in the measurement points and neglecting the process noise in the filters. KF Solid line, RRSQRT-KF dashed-dotted line, and SSQRT-KF dashed line.

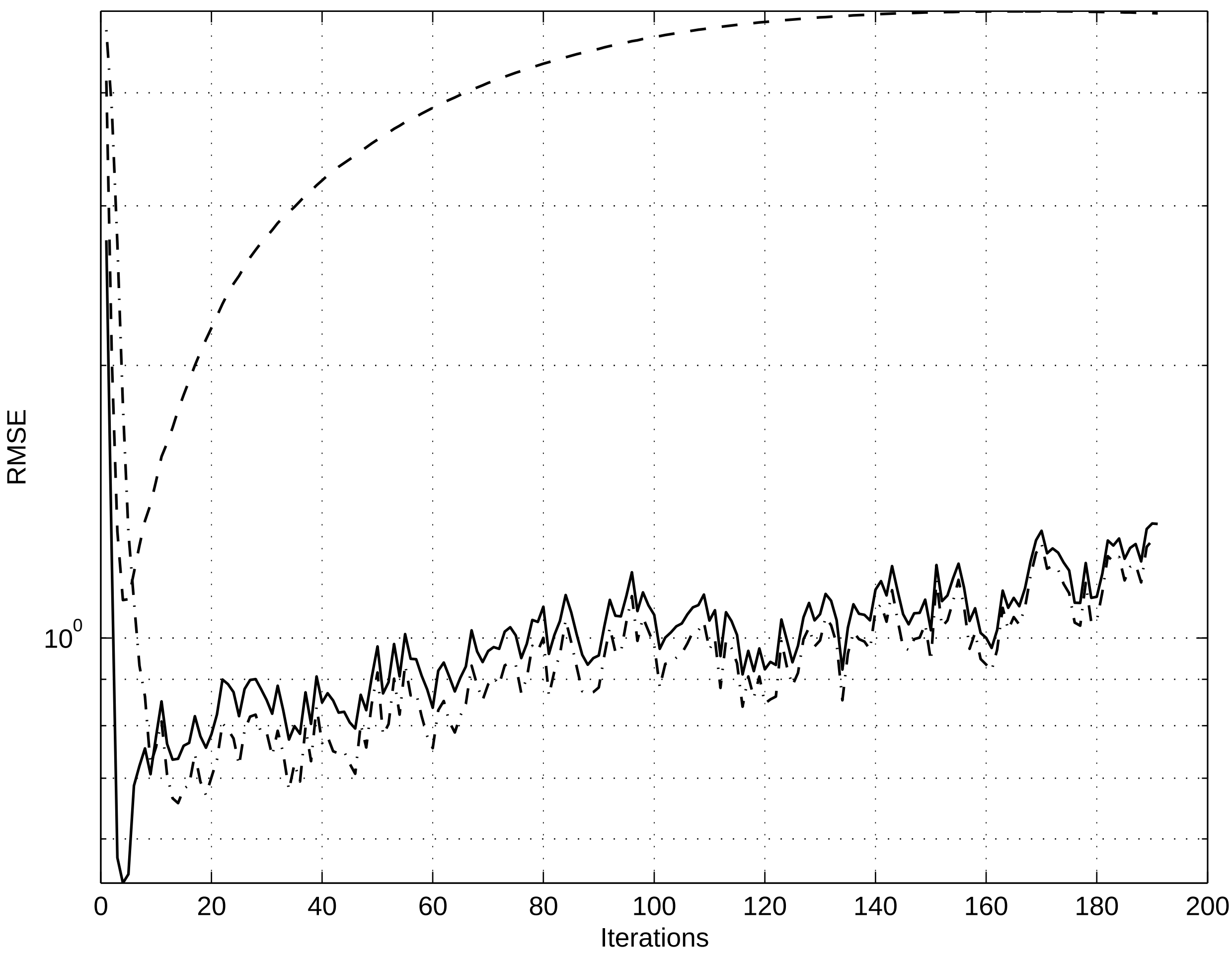

Figure 4: RMSE of $\hat{x}_{k|k}$ for the KF , RRSQRT-KF, and SSQRT-KF, taking just the inputs in the measurement points and adding the process noise to the filters. KF Solid line, RRSQRT-KF dashed-dotted line, and SSQRT-KF dashed line.

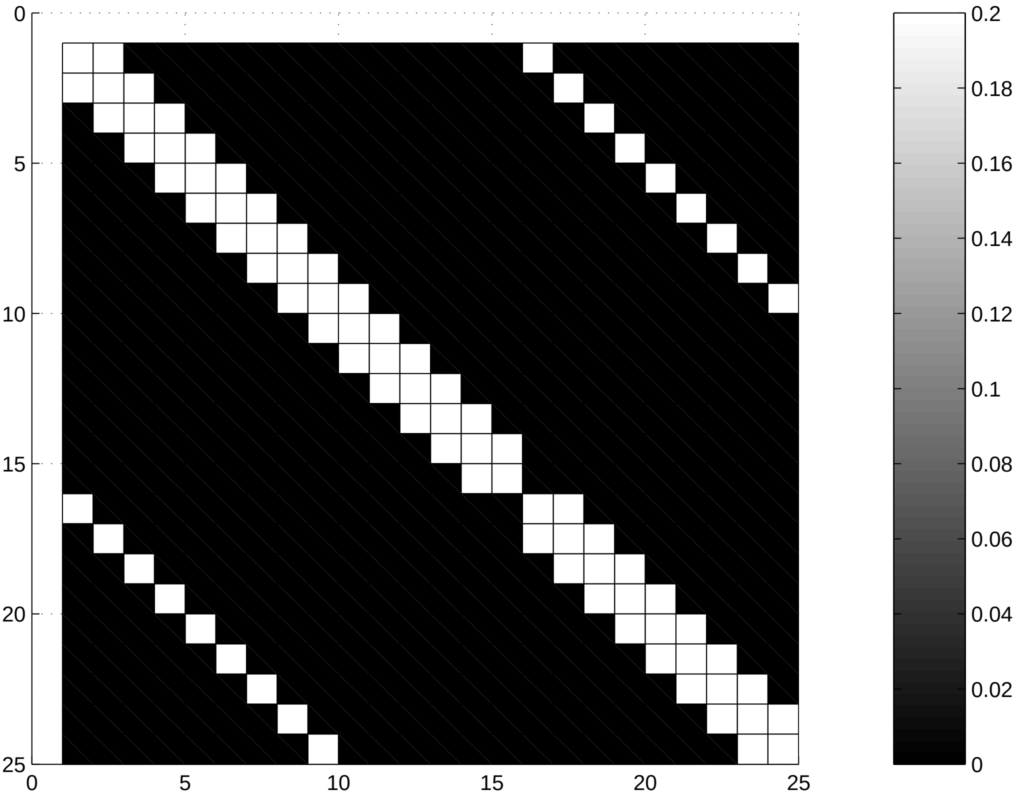

Figure 5: A matrix structure

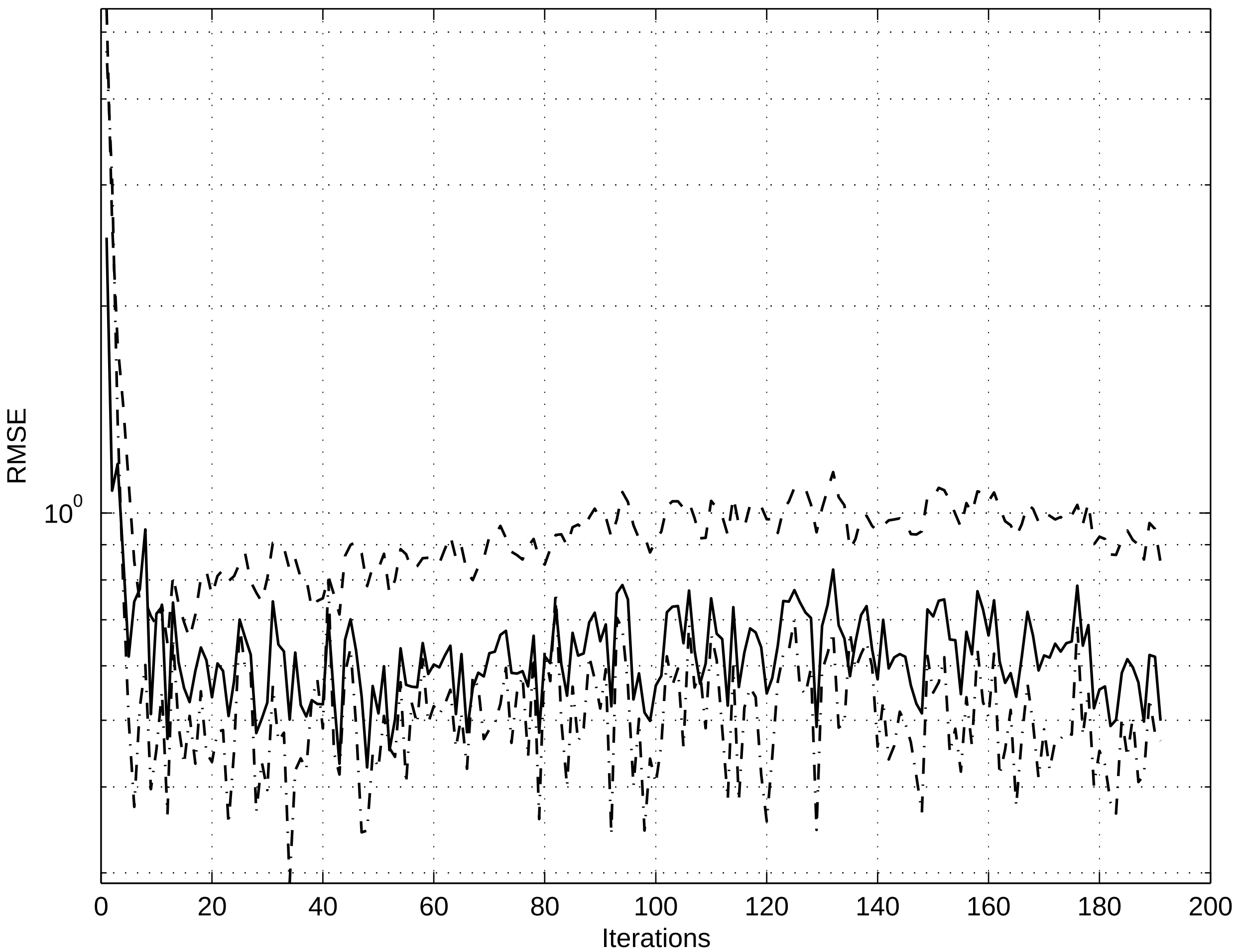

Figure 6: RMSE of $\hat{x}_{k|k}$ for the KF , RRSQRT-KF, and SSQRT-KF, taking just the inputs in the measurement points, adding the process noise to the filters, and using the covariance inflation factor $\gamma = 1.3$. KF Solid line, RRSQRT-KF dashed-dotted line, and SSQRT-KF dashed line.

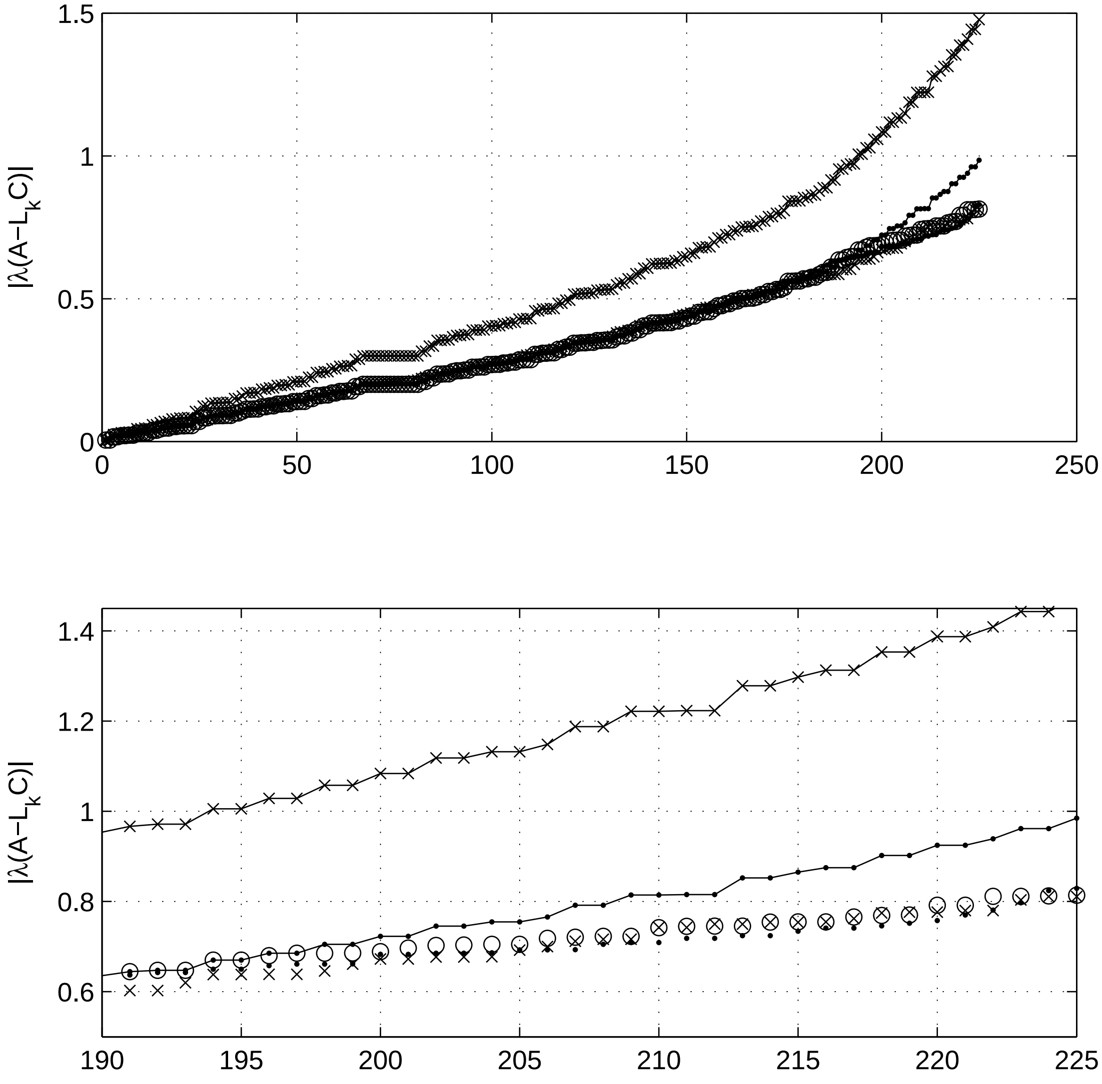

Figure 7: At the top can be seen the eigenvalues of the $(A - L_{kf}C)$, dot-mark, $(A - L_{ks}C)$, circle-mark, $(A - L_{kr})$, x-mark, A, dotted line, and $\tilde{A}$, x-mark line, where L_{kf}, L_{ks}, and L_{kr} are the KF, SSQRT-KF, and RRSQRT-KF gains, respectively. The plot of the bottom depicts how L_{ks} relocates $|\lambda(\tilde{A})| > 1$.

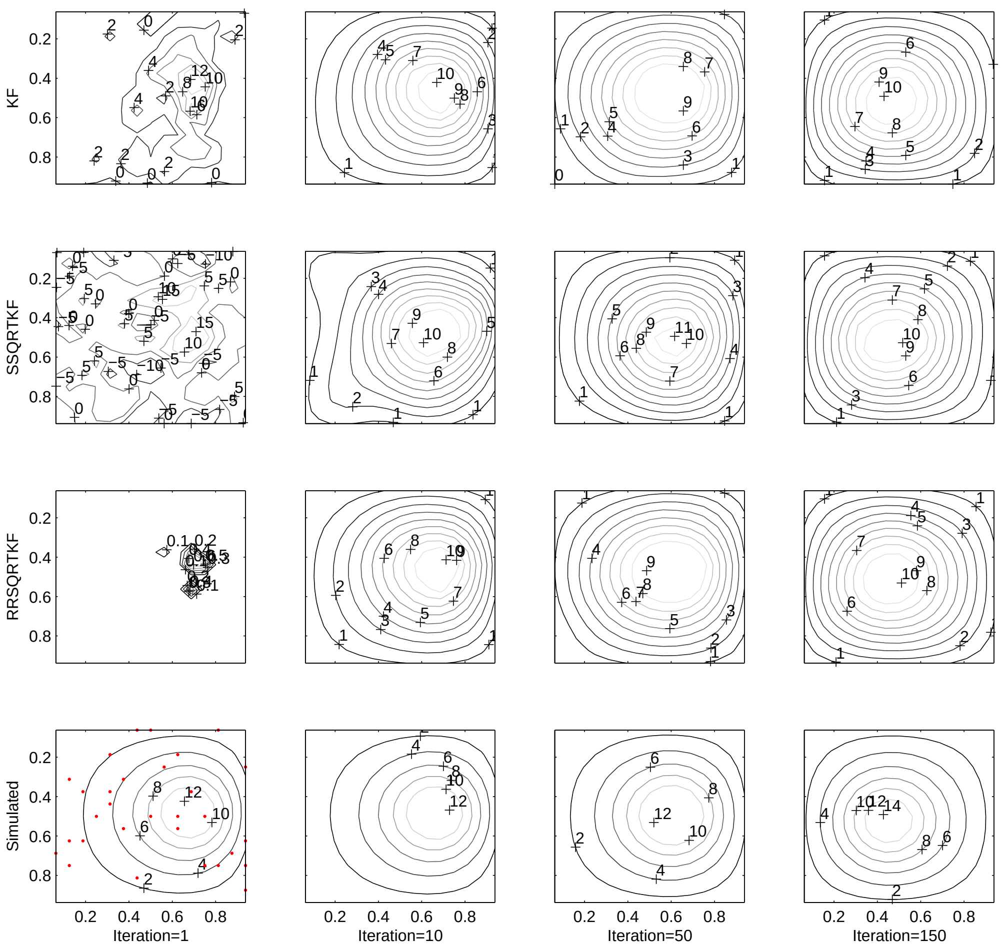

Figure 8: Contour plots of the performance of the three filters compare to the original one (simulated). Taking 30 measurement points (dots in the third row), where the inputs and outputs are measured. Covariance inflation is applied to SSQRT-KF, $\gamma = 1.3$. Random initial conditions and zero fixed boundary conditions.

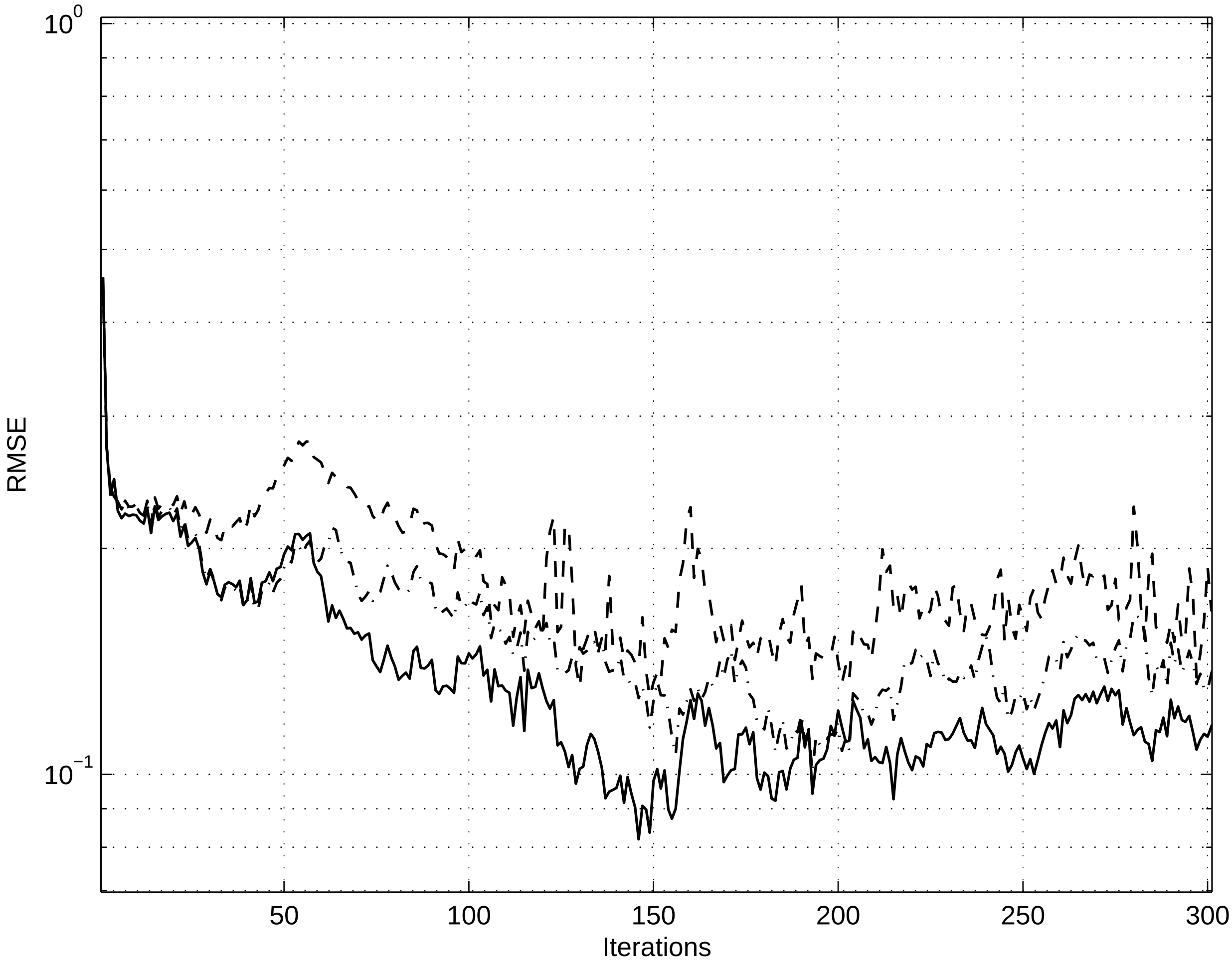

Figure 9: RMSE of $\hat{x}_{k|k}$ for the KF, RRSQRT-KF, and SSQRT-KF. Boundary conditions fixed to zero except the left one, where the disturbance $z_{k+1} = z_k + w_{zk}$ is injected. Randomly 30 measurement points (dots in the third row) were taken, where the outputs are measured. KF Solid line, RRSQRT-KF dashed-dotted line, and SSQRT-KF dashed line.

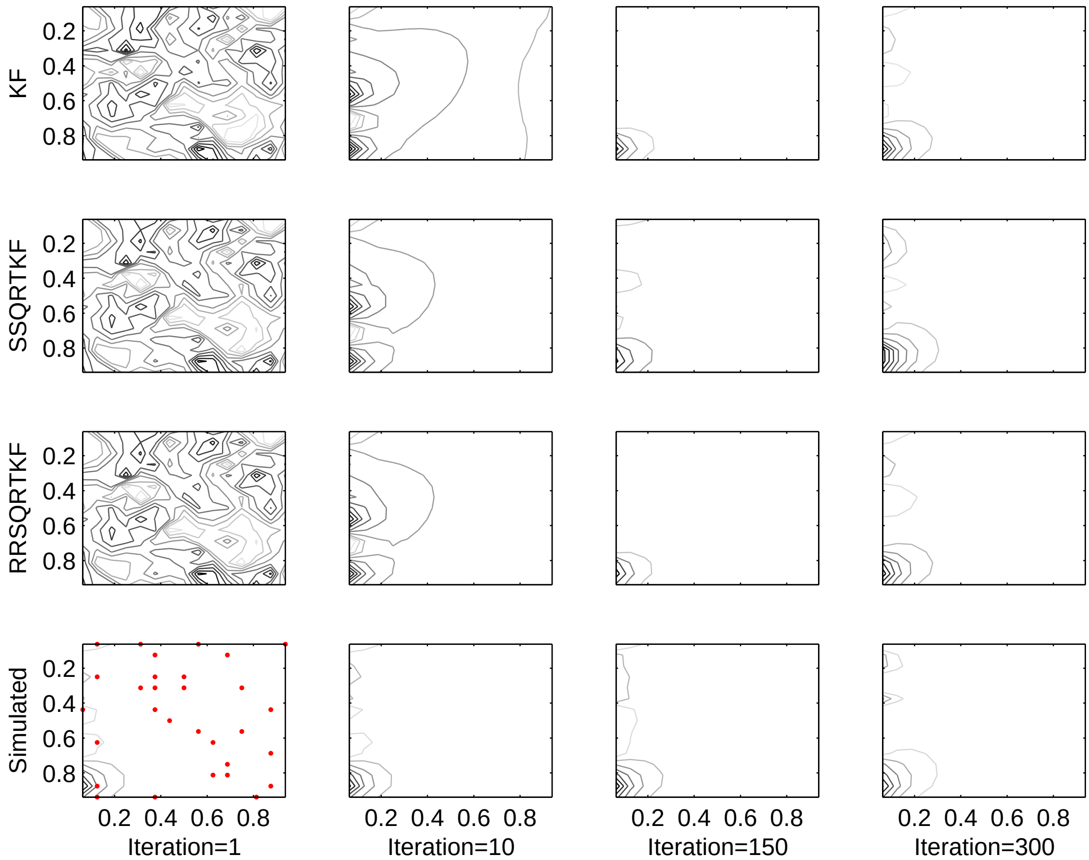

Figure 10: Contour plots of the performance of the three filters compare to the original one (simulated). Boundary conditions fixed to zero except the left one, where the disturbance $z_{k+1} = z_k + w_{zk}$ is injected. Randomly 30 measurement points (dots in the third row) were taken, where the outputs are measured. Covariance inflation is applied to SSQRT-KF, $\gamma = 1.05$. Random initial conditions and zero fixed boundary conditions.